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Note on the determination of the magnetoresistance tensor of a crystal having the symmetry Oh or O

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Note on the determination of the magnetoresistance tensor of a crystal having the symmetry Oh or O

Abstract

In order to get some information about the band structure of conduction electrons or holes it is often desirable to measure the magnetoresistance effect. This note describes a practical method for the determination of the three components of the magnetoresistance tensor for crystals having the point group symmetry Oh or 0 . The methods, which depend upon equations (IIIa), (IIIb) or (IIc) in this note, are most convenient for crystals having a cleavage plane (100), (110) or (111) . In this case, all the tensor components can be obtained by means of a single experimental run.

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NOTE ON THE DETERMINATION OF THE MAGNETORESISTANCE TENSOR OF A CRYSTAL HAVING THE SYMMETRY O_h OR O

by

Toshihiro Okada

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January 1960

Ames Laboratory
at
Iowa State University of Science and Technology
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NOTE ON THE DETERMINATION OF THE MAGNETORESISTANCE TENSOR OF A CRYSTAL HAVING THE SYMMETRY O_h OR O

by

Toshihiro Okada

1. INTRODUCTION

In order to get some information about the band structure of conduction electrons or holes it is often desirable to measure the magnetoresistance effect. This note describes a practical method for the determination of the three components of the magnetoresistance tensor for crystals having the point group symmetry O_h or O. The methods, which depend upon equations (IIIa), (IIIb) or (IIc) in this note, are most convenient for crystals having a cleavage plane (100), (110) or (111). In this case, all the tensor components can be obtained by means of a single experimental run.

2. GENERAL EXPRESSION

According to the thermodynamics of irreversible processes the galvanomagnetic effects of a single crystal are expressed by the following tensor equation[1-3]:

$$E_i = \rho_{ij}\,(\vec{H})\,I_j + \mathcal{E}_{ijk}\,I_j\,R_k\,(\vec{H}), \tag{1}*$$

---

* $\mathcal{E}_{123} = \mathcal{E}_{231} = \mathcal{E}_{312} = -\,\mathcal{E}_{213} = -\,\mathcal{E}_{321} = -\,\mathcal{E}_{132} = 1.$

$\mathcal{E}_{ijk} = 0$, if i = j or k, or j = k.

where E_i and I_j represent, respectively, the components of an electric field applied to the crystal and the components of a current flowing through the crystal. The resistivity tensor $\rho_{ij}(\vec{H})$ is an even function of the magnetic $\vec{H}$ and is equal to $\rho_{ji}(\vec{H})$ because of Onsager's reciprocal relation. $R_k(\vec{H})$ is the Hall vector, which is an odd function of $\vec{H}$.

If the magnetic field is weak $\rho_{ij}(\vec{H})$ and $R_k(\vec{H})$ can be expanded in a power series about the point of zero field as follows:

$$\begin{aligned} \rho_{ij}(\vec{H}) &= \rho_{ij} + \rho_{ijmn} H_m H_n + \ldots\ldots\ldots, \\ R_k(\vec{H}) &= R_{km} H_m + R_{kmno} H_m H_n H_o + \ldots\ldots\ldots, \end{aligned} \tag{2}$$

where

$$\begin{aligned} &\rho_{ij} = \rho_{ji}, \ \rho_{ijmn} = \rho_{jimn} = \rho_{ijnm} = \rho_{jinm}, \\ &R_{kmno} = R_{knmo} = R_{komn} = \ldots\ldots\ldots . \end{aligned} \tag{3}$$

In this note we shall consider only the method for determining ρ_{ijmn} and the method for determining R_{kmno} will not be described here.

In the case of the crystals O_h or O, there is only one non-vanishing constant for ρ_{ij}, three for ρ_{ijmn} and one for R_{km}, as shown in the following two dimensional representations:

$$\rho_{ij} = \begin{pmatrix} \rho_{11} & 0 & 0 \\ 0 & \rho_{11} & 0 \\ 0 & 0 & \rho_{11} \end{pmatrix}, \qquad R_{km} = \begin{pmatrix} R_{11} & 0 & 0 \\ 0 & R_{11} & 0 \\ 0 & 0 & R_{11} \end{pmatrix},$$

$$\rho_{ijmn} = \begin{pmatrix} \rho_{1111} & \rho_{1122} & \rho_{1122} & 0 & 0 & 0 \\ \rho_{1122} & \rho_{1111} & \rho_{1122} & 0 & 0 & 0 \\ \rho_{1122} & \rho_{1122} & \rho_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & \rho_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho_{2323} \end{pmatrix}. \tag{4}$$

If the direction cosines of the current $\vec{I}$ are expressed by $(\beta_1, \beta_2, \beta_3)$, the resistivity is calculated by[(2), (4)]

$$\rho(\vec{H}) = \sum_i \rho_{ii}(\vec{H})\beta_i^2 + 2\sum_{i>j} \rho_{ij}(\vec{H})\beta_i\beta_j . \tag{5}$$

For a weak magnetic field whose direction cosines are $(\alpha_1, \alpha_2, \alpha_3)$, we have

$$\rho(H) = \rho_{11} + H^2 [\rho_{1122} + (\rho_{1111} - \rho_{1122}) \Sigma\alpha_i^2\beta_i^2 + 4\rho_{2323} \sum_{i>j} \alpha_i\alpha_j\beta_i\beta_j], \tag{6}$$

by combining (5) and (4).

We shall consider the following three cases. In each case the current flows along one of the cleavage planes.

Case I. The magnetic field is applied in the plane perpendicular to the direction of the current (see Fig. 1).

Case II. The magnetic field is applied in the plane defined by the direction of the current and by the normal of one of the cleavage planes (see Fig. 2).

Case III. The direction of the magnetic field lies in a cleavage plane (see Fig. 3).

Table I gives the values of $\Sigma\alpha_i\beta_i$, $\Sigma\alpha_i\lambda_i$, $\Sigma\beta_i\lambda_i$ and in each case, the resistance change caused by the magnetic field. λ_i are the direction cosines of the normal $\vec{c}$ of a cleavage plane. As seen from Table I, the main problem is to calculate the values of $\Sigma\alpha_i^2\beta_i^2$.

3. RESULTS

(a) Crystal having a cleavage plane $(\bar{1}00)$.

If we denote the angle between [100] and the direction of $\vec{I}$ by ϕ, we have the following formulas:

$$\frac{\rho(\vec{H}) - \rho_{11}}{H^2} = [\rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \cos^2\phi \sin^2\phi]$$

$$- [(\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \cos^2\phi \sin^2\phi] \cos 2\theta_1,$$

(for Case I)...... (Ia)

$$= \frac{\rho_{1111} + 3\rho_{1122} - 2\rho_{2323}}{4} - \frac{\rho_{1111} - \rho_{1122} - 2\rho_{2323}}{4} \cos 2\theta_1$$

(for Case I, if $\theta_1 = \pi/4$)...... (Ia')

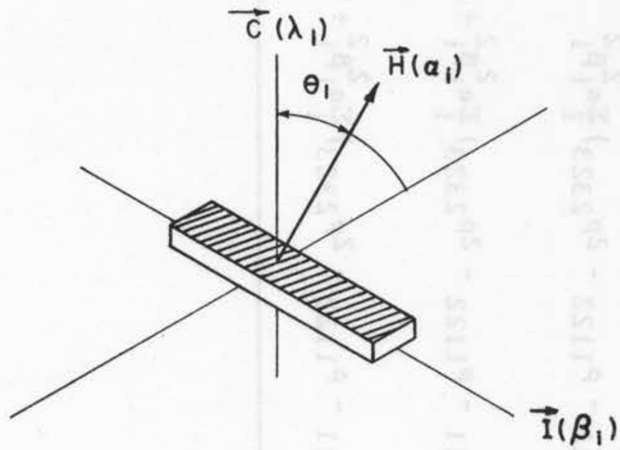

Figure 1

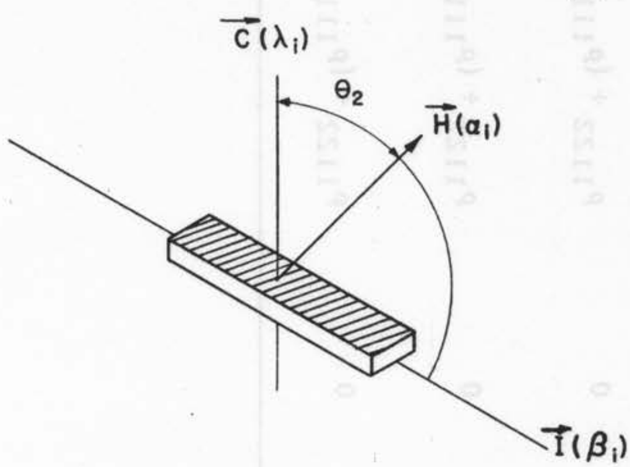

Figure 2

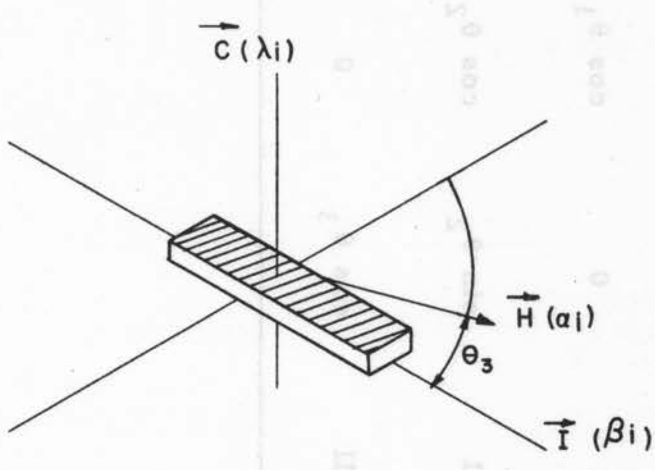

Figure 3

Table I

Case	$\Sigma \alpha_i \beta_i$	$\Sigma \alpha_i \lambda_i$	$\Sigma \beta_i \lambda_i$	$(\rho(\vec{H}) - \rho_{ii})/H^2$
I	0	$\cos\theta_1$	0	$\rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \sum_i \alpha_i^2 \beta_i^2$
II	$\sin\theta_2$	$\cos\theta_2$	0	$\rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \sum_i \alpha_i^2 \beta_i^2 + 2\rho_{2323} \sin^2\theta_2$
III	$\cos\theta_3$	0	0	$\rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \sum_i \alpha_i^2 \beta_i^2 + 2\rho_{2323} \cos^2\theta_3$

$$= \rho_{1122} + \{(\rho_{1111} - \rho_{1122} - 2\rho_{2323})(\cos^4\phi + \sin^4\phi) + 2\rho_{2323}\}\sin^2\theta_2,$$

(for Case II) ....(IIa)

$$= (\rho_{1111} + \rho_{1122})/2 + [\frac{\cos^2 2\phi}{2}(\rho_{1111} - \rho_{1122}) + (1 - \cos^2 2\phi)\rho_{2323}]\cos 2\theta_3$$

$$- [\sin 4\phi/4 \cdot (\rho_{1111} - \rho_{1122} - 2\rho_{2323})]\sin 2\theta_3$$

(for Case III)............(IIIa)

$$= \frac{\rho_{1111} + \rho_{1122}}{2} + \frac{\frac{\rho_{1111} - \rho_{1122}}{2} + \rho_{2323}}{2}\cos 2\theta_3$$

$$- \frac{\frac{\rho_{1111} - \rho_{1122}}{2} - \rho_{2323}}{2}\sin 2\theta_3$$

(for Case III, if $\phi = \pi/8$)....(IIIa')

(IIIa') is one of the most convenient equations for determining the tensor components, because we can obtain the values of $\frac{\rho_{1111} + \rho_{1122}}{2}$, $\frac{\frac{\rho_{1111} - \rho_{1122}}{2} \pm \rho_{2323}}{2}$ (from which we can derive ρ_{1111}, ρ_{1122} and ρ_{2323} very easily) when $\frac{\rho(\vec{H}) - \rho_{11}}{H^2}$ is measured as a function of θ_3. This equation has been used by the author[5] for determing the magnetoresistance tensor of SnTe. Neither (Ia) nor (IIa) is convenient for this purpose, since in both cases the coefficient of $\sin 2\theta$ is zero and hence we obtain only two independent equations involving our three unknowns ρ_{1111}, ρ_{1122}, and ρ_{2323}.

(b) Crystal having a cleavage plane [110].

If we denote the angle between the normal of a cleavage plane and the direction of $\vec{H}$ by θ_1 or θ_2 in Cases I or II respectively and the angle between the current direction and the direction of $\vec{H}$ by θ_3 in Case III, the following expressions are obtained:

$$\frac{\rho(\vec{H}) - \rho_{11}}{H^2} = \rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323})\{3/2 \cdot \sin^2\phi \cos^2\phi \sin^2\theta_1 + 1/2 \cdot \cos^2\phi \cos^2\theta_1\}, \quad \text{(for Case I)} \ldots\ldots\ldots\ldots \text{(Ib)}$$

$$= \rho_{1122} + (\frac{\rho_{1111} - \rho_{1122}}{2} - \rho_{2323}) \cos^2\theta_1, \quad \text{(for Case I, if } \phi = 0) \ldots\ldots\ldots\ldots \text{(Ib')}$$

$$= \rho_{1122}, \quad \text{(for Case I, if } \phi = \pi/2) \ldots\ldots\ldots\ldots \text{(Ib'')}$$

$$= \rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323})\{(\cos^4\phi + 2\sin^4\phi)/2 \cdot \sin^2\theta_2 + 1/2 \cdot \cos^2\phi \cos^2\theta_2\} + 2\rho_{2323} \sin^2\theta_2, \quad \text{(for Case II)} \ldots\ldots\ldots\ldots \text{(IIb)}$$

$$= 1/2 \cdot (\rho_{1111} + \rho_{1122}) - \rho_{2323} \cos 2\,\theta_2$$

(for Case II, if $\phi = 0$).... (IIb')

$$= 1/2 \cdot (\rho_{1111} + \rho_{1122}) - 1/2 \cdot (\rho_{1111} - \rho_{1122}) \cos 2\,\theta_2$$

(for Case II, if $\phi = \pi/2$)...... (IIb'')

$$\begin{aligned} = \rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \{ & (3/8 - 1/8 \cdot \cos 2\phi) \\ & + [3/16 \cdot (1 + \cos 4\phi) - 1/8 \cdot \cos 2\phi] \cos 2\,\theta_3 \\ & + [-3/16 \cdot \sin 4\phi + 1/8 \cdot \sin 2\phi] \sin 2\,\theta_3 \} \\ & + 2\rho_{2323} \cos^2 \theta_3, \end{aligned}$$

(for Case III)............ (IIIb)

$$\begin{aligned} = \frac{11\rho_{1111} - 3\rho_{1122} + 2\rho_{2323}}{8} + \frac{\rho_{1111} - \rho_{1122} - 2\rho_{2323}}{8} \sin 2\,\theta_3 \\ + \rho_{2323} \cos 2\,\theta_3, \end{aligned}$$

(for Case III, if $\phi = \pi/4$)...(IIIb')

Equation (IIIb') is most convenient in practice, since again we can obtain three expressions involving our three unknowns ρ_{1111}, ρ_{1122}, and ρ_{2323}, but no one has used this equation as far as the writer knows.

(c) Crystal having a cleavage plane (111).

If the direction cosines of the current are denoted by $\beta_i (i = 1, 2, 3)$, those of the magnetic field are expressed by the following equations:

$$\alpha_i = \frac{1}{\sqrt{3}} \cos\theta_1 \pm \sqrt{2/3 - \beta_i^2} \sin\theta_1$$

(for Case I)*

* The sign should be selected to satisfy the two equations $\Sigma \alpha_i \beta_i = 0$ and $\Sigma \alpha_i \lambda_i = \cos\theta_1$.

$$= \frac{1}{\sqrt{3}} \cos\theta_2 + \beta_i \sin\theta_2,$$

(for Case II)

where θ_1 or θ_2 is the angle between the normal of a cleavage plane and the direction of the magnetic field. For Case III, it is unnecessary to get the values of α_i as we can calculate the value of $\Sigma\alpha_i^2 \beta_i^2$ in the following way.

From the product of the two equations $\sum_{i>j} \alpha_i \alpha_j = -1/2$ and $\sum_{i>j} \beta_i \beta_j = -1/2$, which are derived from the relation $\Sigma\alpha_i = 0$ and $\Sigma\beta_i = 0$, have

$$1/4 = \sum_{i>j} \alpha_i \alpha_j \beta_i \beta_j + \beta_1 \beta_2 \alpha_3 (\alpha_1 + \alpha_2) + \beta_2 \beta_3 \alpha_1 (\alpha_2 + \alpha_3) + \beta_3 \beta_1 \alpha_2 (\alpha_3 + \alpha_1)$$

$$= \Sigma\alpha_i \alpha_j \beta_i \beta_j - \beta_1 \beta_2 \alpha_3^2 - \beta_2 \beta_3 \alpha_1^2 - \beta_3 \beta_1 \alpha_2^2$$

$$= \sum_{i>j} \alpha_i \alpha_j \beta_i \beta_j - \sum_{i>j} \beta_i \beta_j + \alpha_1^2 \beta_1(\beta_2 + \beta_3) + \alpha_2^2 \beta_2(\beta_1 + \beta_3) + \alpha_2^3 \beta_3(\beta_1 + \beta_2)$$

$$= \sum_{i>j} \alpha_i \alpha_j \beta_i \beta_j + 1/2 - \sum_i \alpha_i^2 \beta_i^2 . \tag{7}$$

On the other hand, from $\Sigma \alpha_i \beta_i = \cos \theta_3$, we get

$$\Sigma \alpha_i \alpha_j \beta_i \beta_j = -1/2 \cdot \Sigma \alpha_i^2 \beta_i^2 + 1/2 \cdot \cos^2 \theta_3 . \tag{8}$$

By comparing the equations (7) and (8), we obtain

$$\Sigma \alpha_i^2 \beta_i^2 = 1/6 + 1/3 \cdot \cos^2 \theta_3 .$$

Hence, we have

$$\frac{\rho(\overrightarrow{H}) - \rho_{11}}{H^2} = \rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \times$$

$$(1/4 + 1/12 \cdot \cos 2\theta_1 + 1/3 \cdot \Sigma (\pm) \sqrt{2/3 - \beta_i^2}\ \beta_i \sin 2\theta_1)$$

$$\text{(for Case I)} \ldots\ldots\ldots\ldots\ldots \text{(Ic)}$$

$$= \frac{5\rho_{1111} + 7\rho_{1122} + 2\rho_{2323}}{12} + \frac{-\rho_{1111} + \rho_{1122} - 10\rho_{2323}}{12} \cos 2\theta_2$$

$$+ (\rho_{1111} - \rho_{1122} - 2\rho_{2323}) \sqrt{3}\, \beta_1 \beta_2 \beta_3 \sin 2\theta_2$$

$$\text{(for Case II)} \ldots\ldots\ldots\ldots\ldots \text{(IIc)*}$$

---

* To get Eq. (IIc), the relations $\Sigma \beta_i^4 = 1/2$ and $\Sigma \beta_i^3 = 3\beta_1 \beta_2 \beta_3$ are used.

$$= \rho_{1122} + (\rho_{1111} - \rho_{1122} - 2\rho_{2323})(1/6 + 1/3 \cdot \cos^2\theta_3) + 2\rho_{2323}\cos^2\theta_3.$$

(for Case III)............ (IIIc)

The equation (IIc) shall be used for the measurement of the tensor components of Mg_2Ge in the near future.

In conclusion, the methods followed by Eqs. (IIIa), (IIIb) and (IIc) seem convenient for the practical measurement of the magnetoresistance tensor.

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